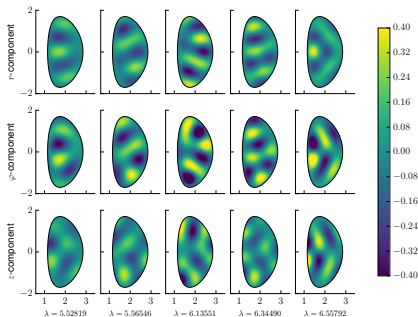


A fast integral equation based solver for the computation of Taylor states in toroidal geometries



Antoine Cerfon, Courant Institute, NYU
with

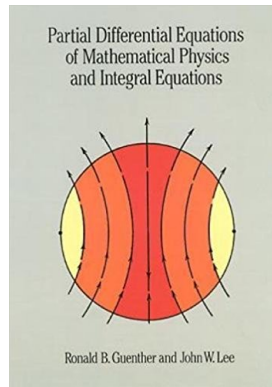
L. Greengard, L.-M. Imbert-Gerard, D. Malhotra, and M. O'Neil

FOREWORD

- ▶ Integral formulations are **our natural way** of thinking as physicists

$$\mathbf{E}(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \int_V \rho(\mathbf{y}) \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|^3} d\mathbf{y}$$

- ▶ Yet, they are **rarely favored by physicists as numerical schemes**
- ▶ Understandable 30 years ago, when key numerical difficulties were unresolved
- ▶ **Applied mathematicians have resolved these issues.** We should now tap the power of integral approaches
- ▶ I will illustrate this with a **new, integral equation based Taylor state solver** designed to be used in SPEC



Chapter 8

OUTLINE

- ▶ Integral equation approaches in physics - advantages, difficulties, and solutions
- ▶ A robust integral formulation for electromagnetic scattering off perfect conductors: the generalized Debye representation for time harmonic Maxwell equations
- ▶ An integral equation based solver for Taylor states in toroidal geometries

Integral equation approaches in physics: advantages, difficulties, and solutions

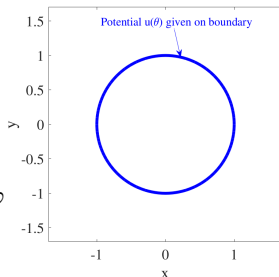
INTEGRAL FORMULATION FOR LAPLACE'S EQUATION

- Compute the potential ϕ inside the disc due to a potential $u(\theta)$ applied on the unit circle
- We learned/worked out in E&M classes that

$$\phi(\mathbf{x}) = -\frac{1}{2\pi} \oint_C \frac{|\mathbf{x}|^2 - 1}{|\mathbf{x} - \mathbf{y}|^2} u(\mathbf{y}) d\mathbf{y}$$
$$\Leftrightarrow \phi(r, \theta) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1 - r^2}{1 + r^2 - 2r \cos(\varphi - \theta)} u(\varphi) d\varphi$$

- For the **exterior Laplace problem**, flip sign in formula

Similar formula for 3D problem and a sphere



INTEGRAL FORMULATION FOR LAPLACE'S EQUATION

Example: $u(\theta) = \cos(30\theta)$

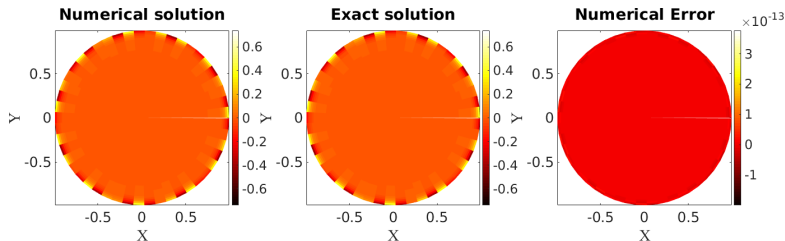
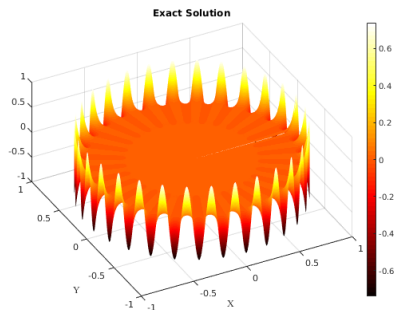
Exact solution:

$$\phi(r, \theta) = r^{30} \cos(30\theta)$$

Use trapezoidal rule for integral.

3000 points on boundary.

Domain discretized with 30 radii
and 30 angles.



INTEGRAL FORMULATIONS - GENERAL FORMALISM

- ▶ Goal: Solve $\Delta\phi = 0$ in Ω with $\phi = u$ on boundary $\partial\Omega$ where Ω is a general 2D domain
- ▶ Green's identity tells us

$$\phi(\mathbf{x}) = -\frac{1}{2\pi} \int_{\partial\Omega} \mathbf{n} \cdot \nabla (\ln |\mathbf{x} - \mathbf{y}|) u(\mathbf{y}) dl_{\mathbf{y}} + \frac{1}{2\pi} \int_{\partial\Omega} \ln |\mathbf{x} - \mathbf{y}| \mathbf{n} \cdot \nabla u(\mathbf{y}) dl_{\mathbf{y}}$$

- ▶ Problem: $\mathbf{n} \cdot \nabla u(\mathbf{y})$ is not known
- ▶ Idea: Look for ϕ of the form

$$\phi(\mathbf{x}) = \int_{\partial\Omega} \mathbf{n} \cdot \nabla (\ln |\mathbf{x} - \mathbf{y}|) \mu(\mathbf{y}) dl_{\mathbf{y}} \quad \text{Double layer potential}$$

- ▶ Continuity of ϕ all the way to $\partial\Omega$ leads to equation for density μ

$$-\frac{1}{2}\mu(\mathbf{x}) + \frac{1}{2\pi} \int_{\partial\Omega} \mathbf{n} \cdot \nabla (\ln |\mathbf{x} - \mathbf{y}|) \mu(\mathbf{y}) dl_{\mathbf{y}} = u(\mathbf{x}) \quad , \quad \mathbf{x} \in \partial\Omega$$

INTEGRAL FORMULATIONS - GENERAL FORMALISM

$$-\frac{1}{2}\mu(\mathbf{x}) + \frac{1}{2\pi} \int_{\partial\Omega} \mathbf{n} \cdot \nabla (\ln |\mathbf{x} - \mathbf{y}|) \mu(\mathbf{y}) d\mathbf{l}_{\mathbf{y}} = u(\mathbf{x}) \quad , \quad \mathbf{x} \in \partial\Omega$$

$$\phi(\mathbf{x}) = \int_{\partial\Omega} \mathbf{n} \cdot \nabla (\ln |\mathbf{x} - \mathbf{y}|) \mu(\mathbf{y}) d\mathbf{l}_{\mathbf{y}}$$

- ▶ Representation as layer potentials leads to **reduction in the dimensionality** of the problem and **great flexibility in the geometry** of the domain
- ▶ Fredholm integral equation of the **second kind** for μ
- ▶ Integral equation **as well-conditioned as the underlying physics**
- ▶ If these equations are discretized with the Nyström method, there is no penalty for over-discretization in terms of stability.

INTEGRAL METHODS IN FUSION – 1976

Stability of a high- β , $l=3$ stellarator

J. P. Freidberg

Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87545

W. Grossmann

Courant Institute of Mathematical Sciences, New York University, New York, New York 10012

F. A. Haas

Culham Laboratory, Abingdon, Oxfordshire, England

(Received 16 March 1976)

The stability of an infinitely long, high β , $l=3$ stellarator is investigated. The calculation is carried out by using the new scyllac expansion in the sharp boundary ideal magnetohydrodynamic model. It is found that for any given size $l=3$ field allowed by equilibrium considerations and mode number m , an infinite but discrete set of wavenumbers k exist for which the plasma is unstable to all β ; that is, the critical β equals zero. These modes can be described as long wavelength interchanges. Thus, with regard to sharp boundary stability, $l=3$ is less desirable than $l=1$ for the basic scyllac magnetic field.

D. Solution of Laplace's equation

We follow closely the procedure outlined previously¹¹ to determine the b_p , \hat{b}_p in terms of the a_p , \hat{a}_p . For this we need the relationship between ψ , $\hat{\psi}$ and $\mathbf{n} \cdot \nabla \psi$, $\mathbf{n} \cdot \nabla \hat{\psi}$ on the plasma surface. This requires the solution of Laplace's equation in the straight helical geometry for the given boundary and prescribed boundary data. The one simplifying feature is that the solution is needed only on the plasma surface and not over the whole domain. The method consists of deriving an integral equation for ψ , $\hat{\psi}$ by using a form of Green's theorem and solving it by Fourier decomposition. As

APPENDIX

Here, we must resolve an important point before a fast and accurate numerical evaluation of the matrix elements A_{pn} and B_{pn} can be carried out. Due to the logarithmic singularity in $F^*(v, v')$ when $v=v'$ a rather large number of grid points would be required for high accuracy. We therefore seek a convenient function to add and subtract from the integrand, such that the two-dimensional fast Fourier transform is applied only to a smooth function.

INTEGRAL METHODS IN FUSION – NESTOR 1986

THREE-DIMENSIONAL FREE BOUNDARY CALCULATIONS USING A SPECTRAL GREEN'S FUNCTION METHOD

S.P. HIRSHMAN, W.I. van RIJ

Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

and

P. MERKEL

Max-Planck-Institut für Plasmaphysik, IPP-EURATOM Association, D-8046 Garching bei München, Fed. Rep. Germany

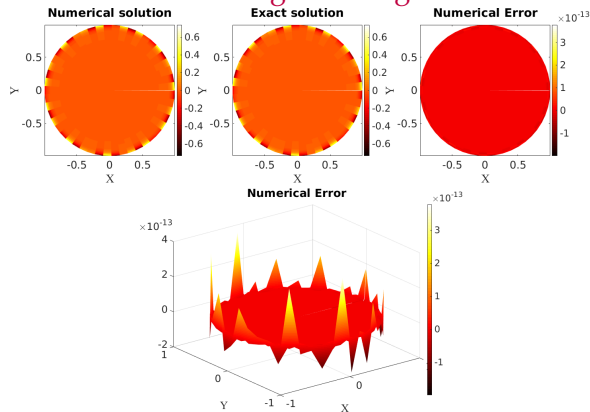
The plasma energy $W_p = \int_{\Omega_p} (\frac{1}{2} B^2 + p) dV$ is minimized over a toroidal domain Ω_p using an inverse representation for the cylindrical coordinates $R = \sum \tilde{R}_{mn}(s) \cos(m\theta - n\xi)$ and $Z = \sum \tilde{Z}_{mn}(s) \sin(m\theta - n\xi)$, where (s, θ, ξ) are radial, poloidal and toroidal flux coordinates, respectively. The radial resolution of the MHD equations is significantly improved by separating R and Z into contributions from even and odd poloidal harmonics which are individually analytic near the magnetic axis. A free boundary equilibrium results when Ω_p is varied to make the total pressure $\frac{1}{2} B^2 + p$ continuous at the plasma surface Σ_p and when the vacuum magnetic field B_v satisfies the Neumann condition $B_v \cdot d\Sigma_p = 0$. The vacuum field is decomposed as $B_v = B_0 + \nabla\Phi$, where B_0 is the field arising from plasma currents and external coils and Φ is a single-valued potential necessary to satisfy $B_v \cdot d\Sigma_p = 0$ when $p \neq 0$. A Green's function method is used to obtain an integral equation over Σ_p for the scalar magnetic potential $\Phi = \sum \Phi_{mn} \sin(m\theta - n\xi)$. A linear matrix equation is solved for Φ_{mn} to determine $\frac{1}{2} B_v^2$ on the boundary. Real experimental conditions are simulated by keeping the external and net plasma currents constant during the iteration. Applications to $l = 2$ stellarator equilibria are presented.

The free boundary problem requires only the value of B_v^2 on the boundary, which is obtained from B_0 and $\Phi(x)$ on Σ_p . Treating the vacuum problem by solving the integral equation (3.2) appears to be an appropriate approach, both because the solution yields $\Phi(x)$ on Σ_p and because no extraneous values of $\Phi(x)$ in the vacuum region are ever computed.

The main difficulty inherent to the Green's function method is the calculation of the Fourier transform of the singular Green's function and its normal derivative. This is solved by the following regularization procedure. Appropriate functions with the same singularity and periodicity are subtracted from the kernels, and their analytically calculated Fourier transforms are added to the Fourier transformed integral equation.

DIFFICULTIES WITH INTEGRAL FORMULATIONS

- Quadratures involve **singular integrands**



- Solving

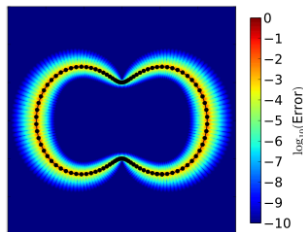
$$-\frac{1}{2}\mu(\mathbf{x}_i) + \frac{1}{2\pi}w_{ij}\mathbf{n} \cdot \nabla (\ln |\mathbf{x}_i - \mathbf{x}_j|) \mu(\mathbf{x}_j) = u(\mathbf{x}_i)$$

in principle $O(N^3)$ work

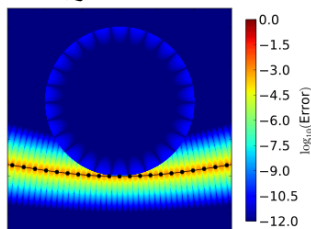
DEALING WITH SINGULAR INTEGRANDS: QBX

- ▶ Field induced by integral operator is **locally smooth when restricted to the interior**
- ▶ Idea: Take expansion centers away from $\partial\Omega$ and evaluate field close to $\partial\Omega$ through Taylor expansions
- ▶ Known as **Quadrature By Expansion (QBX)** scheme¹ (QBX) scheme

Standard Trapezoidal



QBX

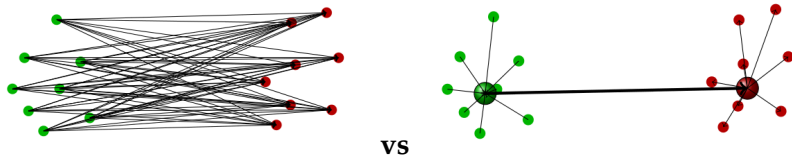


¹A. Klöckner, A. Barnett, L. Greengard and M. O'Neil, *J. Comp. Phys* **252**, 332 (2013)

ACCELERATING THE CALCULATION OF μ

A seemingly unrelated problem: Consider N charges q_i at different locations \mathbf{z}_i , and compute the potential ϕ at each \mathbf{z}_i

- ▶ A naive calculation takes $O(N^2)$ work.
- ▶ Can do much better: think of two separate groups of charges



- ▶ Idea of the **Fast Multipole Method**²: Approximate potential far away from given group of charges by multipole expansion

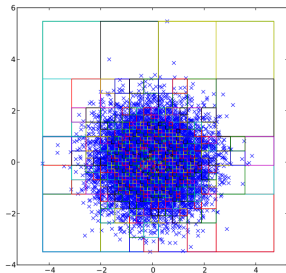
$$\phi(\mathbf{z}) = \left(\sum_i^N q_i \right) \ln \mathbf{z} + \sum_{k=1}^{\infty} \frac{a_k}{\mathbf{z}^k} \quad a_k = - \sum_{i=1}^N \frac{q_i \mathbf{z}_i}{k}$$

- ▶ Accuracy determined by number of terms p in expansion and minimal distance between groups of charges

²L. Greengard and V. Rokhlin, *J. Comp. Phys.* **73**, 325 (1987)

THE FAST MULTIPOLE METHOD FOR POINT CHARGES

- For given charge distribution, construct adaptive quad tree



- Define adjacent boxes as neighbors
- For neighbors, compute interaction with exact summation
- For boxes far away, use expansion - accuracy now only depends on p
- Run time complexity: $O(N)$!

THE FMM FOR THE COMPUTATION OF μ

- ▶ The FMM can be viewed as a **fast scheme for evaluating the matrix vector product**

$$\phi = M\mathbf{q}$$

with $M_{ij} = 1/2\pi \ln |\mathbf{x}_i - \mathbf{x}_j|$ and \mathbf{q} the vector of point charges

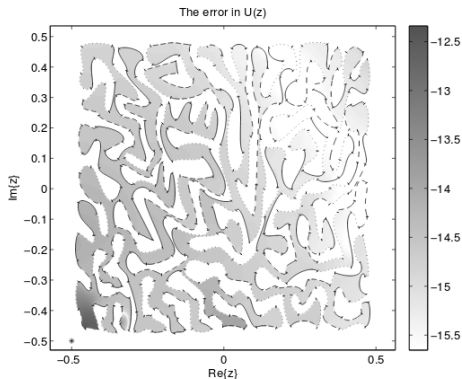
- ▶ Matrix equation for μ is $(\mathbf{I} - \mathbf{K})\mu = -2\mathbf{u}$ with \mathbf{K} in the class of operators for which FMM works
- ▶ μ can be solved in order **N or $N \log N$ time** with FMM+GMRES
- ▶ Recently, new **fast direct solvers** developed, which can be competitive^{3,4}
- ▶ Often, high accuracy reached for N small, so dense linear algebra does not hurt

³K.L. Ho, L. Greengard, *SIAM J. Sci. Comput.* **34**, A2507A2532 (2012)

⁴S. Ambikasaran and E. Darve, *SIAM J. Sci. Comput.* **57**, 477 (2013)

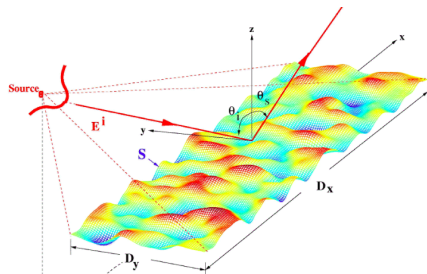
INTEGRAL FORMULATIONS HAVE DEFEATED LAPLACE'S EQUATION

Example: R. Ojala and J. Helsing (2011)



A robust integral formulation for electromagnetic scattering off perfect conductors: the generalized Debye sources representation for time harmonic Maxwell equations

ELECTROMAGNETIC SCATTERING



- Time-harmonic problem:

$$\nabla \times \mathbf{H} = -ik\mathbf{E} \quad , \quad \nabla \times \mathbf{E} = ik\mathbf{H}$$

- Subject to perfect conductor boundary conditions:

$$\mathbf{n} \times \mathbf{E} = \mathbf{0} \quad , \quad \mathbf{n} \cdot \mathbf{H} = 0$$

INTEGRAL FORMULATIONS FOR TIME-HARMONIC MAXWELL

$$\mathbf{E} = ik\mathbf{A} - \nabla\phi \quad , \quad \mathbf{H} = \nabla \times \mathbf{A}$$

with

$$\mathbf{A}(\mathbf{x}) = \int_{\Gamma} \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \mathbf{J}(\mathbf{y}) dA_{\mathbf{y}} \quad , \quad \phi(\mathbf{x}) = \frac{1}{ik} \int_{\Gamma} \frac{e^{ik|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} (\nabla_{\Gamma} \cdot \mathbf{J})(\mathbf{y}) dA_{\mathbf{y}}$$

Two formulations usually considered:

1. **Electric Field Integral Equation Formulation (EFIE)**: unknown is \mathbf{J} , and integral equation for \mathbf{J} obtained by imposing $\mathbf{n} \times \mathbf{E} = \mathbf{0}$
2. **Magnetic Field Integral Equation Formulation (MFIE)**: unknown is \mathbf{J} , and integral equation for \mathbf{J} obtained by imposing $\mathbf{n} \times \mathbf{H} = \mathbf{J}$

ISSUES WITH EFIE AND MFIE

- ▶ Both formulations have **spurious resonances**: frequencies k for which the **integral equations are not invertible**
- ▶ **“Low frequency breakdown”**: \mathbf{E} involves one term $\propto k$ and one term $\propto 1/k$
- ▶ The electric field does not uncouple naturally from the magnetic field as $k \rightarrow 0$
- ▶ In the multiply connected case, the MFIE has a nontrivial null space in the limit $k \rightarrow 0$

AN ELEGANT SOLUTION: THE GENERALIZED DEBYE REPRESENTATION

- Use **potentials** (\mathbf{A}, u) and **antipotentials** (\mathbf{Q}, v) to write \mathbf{E} and \mathbf{H} ⁵:

$$\mathbf{E} = ik\mathbf{A} - \nabla u - \nabla \times \mathbf{Q} \quad , \quad \mathbf{H} = ik\mathbf{Q} - \nabla v + \nabla \times \mathbf{A}$$

with

$$\begin{aligned} \mathbf{A}(\mathbf{x}) &= \int_{\Gamma} \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \mathbf{j}(\mathbf{x}') dA' & u(\mathbf{x}) &= \int_{\Gamma} \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} r(\mathbf{x}') dA' \\ \mathbf{Q}(\mathbf{x}) &= \int_{\Gamma} \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \mathbf{m}(\mathbf{x}') dA' & v(\mathbf{x}) &= \int_{\Gamma} \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \sigma(\mathbf{x}') dA' \end{aligned}$$

with the continuity conditions $\nabla_{\Gamma} \cdot \mathbf{j} = ikr$, $\nabla_{\Gamma} \cdot \mathbf{m} = ik\sigma$

- In the simply connected case, system of equations has a **unique solution for all frequencies with nonnegative imaginary part**
- **Uncoupling** into an **electrostatic problem** involving r and a **magnetostatic problem** involving σ in **limit** $k \rightarrow 0$

⁵C.L. Epstein, L. Greengard, and M. O'Neil. "Debye Sources, Beltrami Fields, and a Complex Structure on Maxwell Fields", *CPAM* **68**, 2237–2280 (2016)

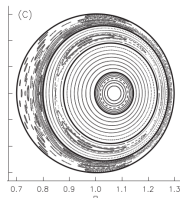
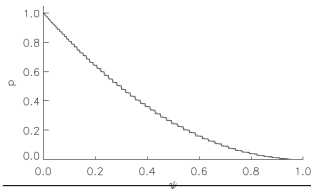
An integral equation based solver for Taylor states in toroidal geometries

STELLARATOR EQUILIBRIA AND BELTRAMI FIELDS

- **Proof of existence of 3D MHD equilibria for piecewise constant pressure profile** (and small departure from axisymmetry) by O.P. Bruno and P. Laurence, *CPAM* **49**, 717 (1996)
- Magnetic field in torii with constant pressure:

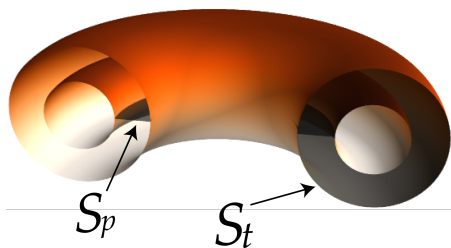
$$\nabla p = 0 \Rightarrow \mathbf{J} = \mu \mathbf{B} \Rightarrow \nabla \times \mathbf{B} = \lambda \mathbf{B} \quad \text{Beltrami field!}$$

- Such equilibria also make physical sense (*Taylor relaxation*) and form the basis of the code SPEC⁶



⁶S. R. Hudson, R. L. Dewar, G. Dennis, M. J. Hole, M. McGann, G. von Nessi, and S. Lazerson, *PoP* **19**, 112502 (2012)

BELTRAMI FIELDS THROUGH GENERALIZED DEBYE POTENTIALS



Given $\lambda, \Phi_{tor}, \Phi_{pol}$, solve

$$\left\{ \begin{array}{ll} \nabla \times \mathbf{B} = \lambda \mathbf{B} & \text{in } \Omega \\ \mathbf{B} \cdot \mathbf{n} = 0 & \text{on } \Gamma \\ \int_{S_t} \mathbf{B} \cdot d\mathbf{S} = \Phi_{tor}, \int_{S_p} \mathbf{B} \cdot d\mathbf{S} = \Phi_{pol} \end{array} \right.$$

- ▶ Let $\mathbf{E} = i\mathbf{B}$, $\mathbf{H} = \mathbf{B}$ satisfy the **vacuum time-harmonic Maxwell equations**, with λ playing the role of k
- ▶ General potentials/“antipotentials” representation for \mathbf{E} and \mathbf{H}

$$\mathbf{E} = i\lambda \mathbf{A} - \nabla u - \nabla \times \mathbf{Q}$$

$$\mathbf{H} = i\lambda \mathbf{Q} - \nabla v + \nabla \times \mathbf{A}$$

- ▶ Satisfy $\mathbf{E} = i\mathbf{H}$ if $\mathbf{A} = i\mathbf{Q}$, $u = iv$. Write \mathbf{B} as

$$\mathbf{B} = i\lambda \mathbf{Q} - \nabla v + i\nabla \times \mathbf{Q}$$

GENERALIZED DEBYE REPRESENTATION OF \mathbf{Q} AND v

- \mathbf{Q} and v are written in terms of layer potentials

$$\mathbf{Q}(\mathbf{x}) = \int_{\Gamma} \frac{e^{i\lambda|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \mathbf{m}(\mathbf{x}') dA' \quad v(\mathbf{x}) = \int_{\Gamma} \frac{e^{i\lambda|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \sigma(\mathbf{x}') dA'$$

- \mathbf{m} and σ are related through

$$\mathbf{m} = i\lambda \left(\nabla_{\Gamma} \Delta_{\Gamma}^{-1} \sigma - i \mathbf{n} \times \nabla_{\Gamma} \Delta_{\Gamma}^{-1} \sigma \right) + \alpha \mathbf{m}_H.$$

∇_{Γ} : surface gradient operator

Δ_{Γ}^{-1} : inverse of the surface Laplacian along Γ restricted to the class of *mean-zero functions*

\mathbf{m}_H is a tangential harmonic vector field satisfying

$$\nabla_{\Gamma} \cdot \mathbf{m}_H = 0, \quad \nabla_{\Gamma} \cdot \mathbf{n} \times \mathbf{m}_H = 0 \quad \mathbf{n} \times \mathbf{m}_H = -i \mathbf{m}_H.$$

α : complex number determined by B.C.

INTEGRAL EQUATION FOR σ AND α

- Apply $\mathbf{B} \cdot \mathbf{n} = 0$ and the flux condition to get integral equations for σ and α :

$$\begin{aligned} \frac{\sigma}{2} - \mathbf{n} \cdot \nabla \int_{\Gamma} \frac{e^{i\lambda|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \sigma(\mathbf{x}') dS' \\ + i\lambda \mathbf{n} \cdot \int_{\Gamma} \frac{e^{i\mu|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \mathbf{m} dS' + i\mathbf{n} \cdot \nabla \times \int_{\Gamma} \frac{e^{i\lambda|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \mathbf{m} dS' = 0 \end{aligned}$$

$$\frac{1}{\mu} \int_{\partial S_t} \mathbf{B} \cdot d\mathbf{l} = \Phi^{tor}$$

- Well-conditioned, second kind integral equation
- Unknowns only defined on Γ
- Similar formulation (with more terms) for toroidal *shells*

NUMERICS

- ▶ 16th order hybrid Gauss-trapezoidal rule for singular integrals
- ▶ Use Fourier spectral differentiation matrix to evaluate ∇_Γ
- ▶ Compute Δ_Γ^{-1} by solving

$$(\Delta_\Gamma + \int_\Gamma dS)\omega = f$$

Invertible equation, and ω satisfies $\Delta_\Gamma \omega = f$ and $\int_\Gamma \omega dS = 0$

- ▶ Use recent numerical scheme for \mathbf{m}_H for nonaxisymmetric surfaces⁷
- ▶ Major simplifications for axisymmetric equilibria:
 1. Closed form formula for basis of harmonic surface vector field \mathbf{m}_H

$$\mathbf{m}_{H_1} = \frac{1}{R}\boldsymbol{\tau} \quad \mathbf{m}_{H_2} = -\frac{1}{R}\mathbf{e}_\zeta$$

where $\boldsymbol{\tau}, \mathbf{e}_\zeta, \mathbf{n}$ local orthonormal basis on flux surface.

2. High order accuracy achieved with few unknowns \Rightarrow dense linear algebra solvers fast

⁷L.-M. Imbert-Gérard, L. Greengard, Numerical Methods for PDEs, **33** 941 (2017)

TESTING THE SOLVER: CONSTRUCTING EXACT TAYLOR STATES ⁸

- View Taylor state as **Grad-Shafranov equilibrium**

$$\Delta^* \psi = -\lambda^2 \psi \quad \text{in } \Omega, \quad \psi = 0 \quad \text{on } \Gamma$$

- A general solution is

$$\psi(r, z, c_1, c_2, c_3, c_4, c_5, c_6, \lambda) = \psi_0 + c_1 \psi_1 + c_2 \psi_2 + c_3 \psi_3 + c_4 \psi_4 + c_5 \psi_5$$

$$\psi_0 = rJ_1(\lambda r), \quad \psi_1 = rY_1(\lambda r), \quad \psi_2 = rJ_1\left(\sqrt{\lambda^2 - c_6^2}r\right) \cos(c_6 z)$$

$$\psi_3 = rY_1\left(\sqrt{\lambda^2 - c_6^2}r\right) \cos(c_6 z), \quad \psi_4 = \cos\left(\lambda\sqrt{r^2 + z^2}\right)$$

$$\psi_5 = \cos(\lambda z)$$

- The toroidal flux is then given by $\Phi^{tor} = \lambda \iint_{\Omega} \frac{\psi}{r} dr dz$
- For Taylor states with **X-points**, use 5 more terms and 5 more c_i

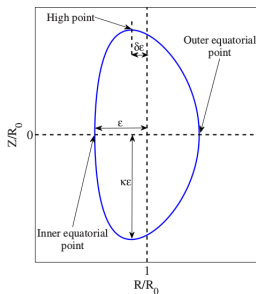
⁸A.J. Cerfon and M. O'Neil, "Exact axisymmetric Taylor states for shaped plasmas", *Phys. Plasmas* **21**, 064501 (2014)

TESTING THE SOLVER: CONSTRUCTING EXACT TAYLOR STATES

- Treat λ as unknown along with the 6 c_i
- Solve for the unknowns by imposing 7 conditions on $\psi = 0$ curve

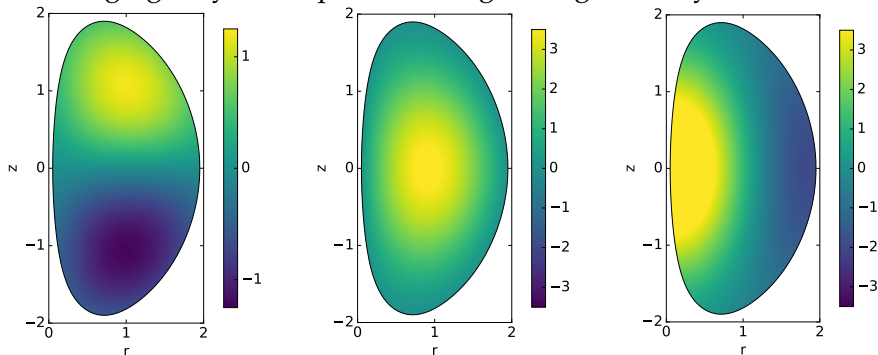
$$\left\{ \begin{array}{l} \psi(1 + \epsilon, 0, C) = 0 \\ \psi(1 - \epsilon, 0, C) = 0 \\ \psi(1 - \delta\epsilon, -\kappa\epsilon, C) = 0 \\ \psi_r(1 - \delta\epsilon, -\kappa\epsilon, C) = 0 \\ \psi_{zz}(1 + \epsilon, 0, C) + N_1\psi_r(1 + \epsilon, 0, C) = 0 \\ \psi_{zz}(1 - \epsilon, 0, C) + N_2\psi_r(1 - \epsilon, 0, C) = 0 \\ \psi_{rr}(1 - \delta\epsilon, -\kappa\epsilon, C) + N_3\psi_z(1 - \delta\epsilon, -\kappa\epsilon, C) = 0 \end{array} \right.$$

N_1, N_2, N_3 : curvatures at three points $(1 + \epsilon, 0)$, $(1 - \epsilon, 0)$, $(1 - \delta\epsilon, \kappa\epsilon)$



COMPARISON WITH EXACT BELTRAMI FIELD

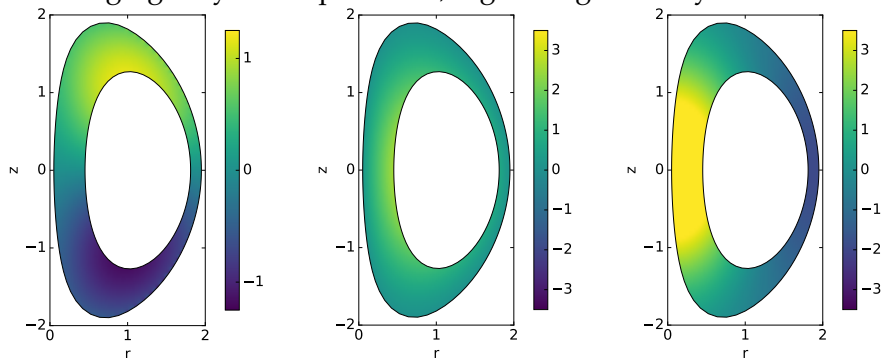
Challenging very low aspect ratio, high elongation Taylor state:



n	B_r	B_ϕ	B_z	$ \mathbf{B} - \mathbf{B}_{\text{exact}} / \mathbf{B}_{\text{exact}} $
25	0.443052524078644	3.10056763474524	-3.784408049008867E-002	$2.7 \cdot 10^{-3}$
50	0.442014263551259	3.09845144534915	-4.109405171821609E-002	$2.5 \cdot 10^{-5}$
100	0.442018001760211	3.09850436011175	-4.104126312770094E-002	$3.9 \cdot 10^{-8}$
200	0.442017994270342	3.09850428092008	-4.104130814605825E-002	$1.2 \cdot 10^{-8}$

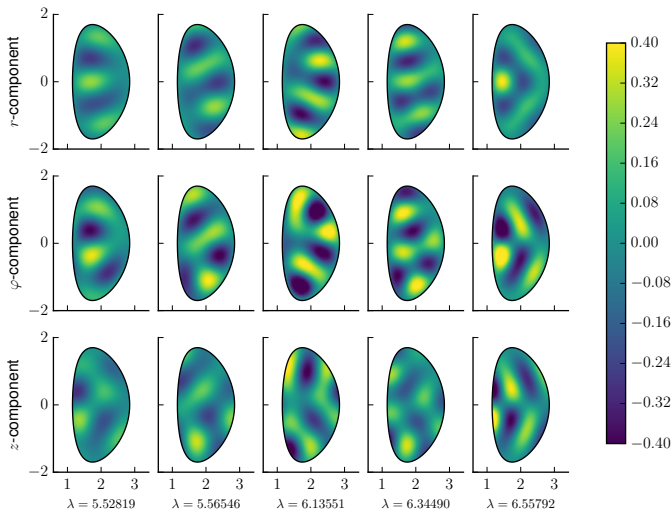
COMPARISON WITH EXACT BELTRAMI FIELD

Challenging very low aspect ratio, high elongation Taylor state:



n	B_r	B_ϕ	B_z	$ \mathbf{B} - \mathbf{B}_{\text{exact}} / \mathbf{B}_{\text{exact}} $
25	-0.7790590773628590	0.5058371725845370	0.9957374643442100	$1.3 \cdot 10^{-2}$
50	-0.7758504363890280	0.5043487336557070	0.9869834030024680	$7.3 \cdot 10^{-4}$
100	-0.7754614741802320	0.5046765566326400	0.9867586238268730	$3.0 \cdot 10^{-6}$
200	-0.7754611961412940	0.5046760189196530	0.9867575110491060	$8.6 \cdot 10^{-7}$

BELTRAMI RESONANCES



$N = 1$ non-axisymmetric Taylor states for $\lambda \in [1, 8]$

RECAP

- ▶ We developed an integral equation formulation for Taylor states in toroidal geometries
- ▶ $\nabla \times \mathbf{B} = \mu \mathbf{B}$ **exactly, by construction**, independently of the accuracy of the answer
- ▶ Unknowns **only defined on the boundary of the domain**
- ▶ Reduction in dimension \Rightarrow **high accuracy for low number of unknowns**, and **low memory requirement**
- ▶ Particularly interesting for SPEC, since at each iteration step, **$B^2/2\mu_0 + p$ only needed on boundary of each region**
- ▶ Exploring additional savings for the iteration, because of theorem by Kirsch regarding boundary derivatives in scattering problems⁹
- ▶ Code for general stellarator geometries finished by December

⁹A. Kirsch, The domain derivative and two applications in inverse scattering theory, *Inverse Problems* **9** 81 (1993)

Integral equation approaches in physics: advantages, difficulties, and solutions

GRAD-SHAFRANOV EQUATION AS NONLINEAR POISSON PROBLEM

$$R \frac{\partial}{\partial R} \left(\frac{1}{R} \frac{\partial \Psi}{\partial R} \right) + \frac{\partial^2 \Psi}{\partial Z^2} = R^2 h(\Psi(R, Z), R)$$

- ▶ Solution requires **iteration** as we saw
- ▶ Without extra computational cost, solve GSE as

$$\frac{\partial^2 \Psi}{\partial R^2} + \frac{\partial^2 \Psi}{\partial Z^2} = \frac{1}{R} \frac{\partial \Psi}{\partial R} + R^2 h(\Psi(R, Z), R)$$

Pro: Gives access to numerical methods for Poisson's equation

Con: Iteration on derivative term converges less fast

- ▶ **Better solution**, change unknown: $\Psi = \sqrt{R}U$

$$\frac{\partial^2 U}{\partial R^2} + \frac{\partial^2 U}{\partial Z^2} = \frac{3}{4} \frac{U}{R^2} + R^{3/2} h(\sqrt{R}U, R)$$

$$U = 0 \quad \text{on plasma boundary}$$